

TECHNICAL DATA SHEET

ALLYL HEXANOATE

Fruity aroma chemical with a pronounced pineapple and tropical-fruit character

1. RAW MATERIAL IDENTIFICATION

Product name	Allyl Hexanoate
Synonyms	Allyl Caproate; Allyl n-Caproate; 2-Propenyl Hexanoate; Hexanoic Acid Allyl Ester
INCI name	ALLYL CAPROATE
CAS number	123-68-2
EC number	204-642-4
FEMA number	2032
IUPAC name	Prop-2-en-1-yl hexanoate
Molecular formula	$C_9H_{16}O_2$
Molecular weight	156.22 g/mol
Chemical group	Aliphatic ester; allyl ester of hexanoic acid
Raw material origin	Usually synthetic; natural origin must be confirmed by the manufacturer's documentation
Raw material category	Aroma chemical

2. OLFACTORY CLASSIFICATION AND ODOUR PROFILE

Fragrance note	Top note
Primary olfactory family	Fruity – Non Citrus
Secondary olfactory family	Gourmand – Sweet
Odour profile	Intense, sweet and fruity, with a dominant pineapple note and tropical, rum-like and slightly fatty nuances

Allyl Hexanoate is an aroma chemical with a powerful, sweet and distinctly fruity odour profile. Its dominant olfactory feature is the recognisable aroma of fresh, juicy pineapple, accompanied by nuances of tropical fruit, rum, arrack, cognac and a slightly fatty-fruity facet.

TECHNICAL DATA SHEET

3. DESCRIPTION AND FUNCTION IN FRAGRANCE COMPOSITION

Compared with Allyl Amyl Glycolate, Allyl Hexanoate produces a sweeter, juicier and more immediate pineapple effect. It is less green and galbanum-like, but more distinctly tropical, fermented and rum-like. It is therefore one of the fundamental aroma chemicals used to construct pineapple and mixed tropical-fruit accords.

The material has a powerful initial odour impact but relatively short olfactory persistence. It is most pronounced in the opening of a composition, where it provides juiciness, sweetness and tropical freshness. At excessive concentrations, it may develop a sharp, fatty, overripe or distinctly synthetic fruity character.

4. APPLICATION AND OLFATORY COMPATIBILITY

Allyl Hexanoate is primarily used to build and enhance fruity top notes. Its principal role is the construction of pineapple accords, although it is also used in apple, apricot, peach, banana, strawberry, orange and other tropical-fruit accords.

Suitable for:

- fruity and tropical fragrance compositions;
- pineapple accords;
- citrus-fruity and floral-fruity fragrances;
- apple, peach, apricot and strawberry accords;
- rum, cognac and liqueur accords;
- soaps and washing products;
- air fresheners and other functional fragrance products.

It combines well with ethyl butyrate, ethyl hexanoate, isoamyl acetate, allyl heptanoate and other fruity esters, as well as citrus oils, aldehydes, green notes, jasmine materials, lactones, vanilla materials and light woody notes.

In green and mossy compositions, it can be used as a contrasting note that softens dryness and introduces a juicy fruity nuance. Combined with citrus notes, it contributes a sweeter and more distinctly tropical character.

5. RECOMMENDED USE

Typical use level in fragrance concentrate	Approximately 0.01–1.00%
0.01–0.10%	Subtle fruity freshness and juiciness
0.10–0.50%	Clearly expressed pineapple and tropical-fruit note
0.50–1.00%	Dominant pineapple or mixed tropical-fruit accord
Pre-dilution	10% solution in DPG or ethanol for easier and more precise dosing

The stated ranges are indicative perfumery use levels, not regulatory maximum concentrations. The permitted concentration in the finished product must be verified against the current IFRA Standard, the documentation of the specific manufacturer and the applicable finished-product category.

TECHNICAL DATA SHEET

6. PHYSICOCHEMICAL AND TECHNICAL DATA

Appearance	Clear liquid
Colour	Colourless to pale yellow
Odour	Intense, sweet and fruity, with a dominant pineapple note and tropical, rum-like and slightly fatty nuances
Relative density	Approximately 0.884-0.892
Refractive index at 20 °C	Approximately 1.422-1.426
Boiling point	Approximately 186-191 °C
Flash point	Approximately 63-66 °C, closed-cup method
Solubility	Practically insoluble in water; soluble in ethanol, oils and common organic perfumery solvents
Volatility	Moderately high; pronounced initial impact and relatively short olfactory persistence

The stated density, refractive-index, boiling-point and flash-point values are standard approximate ranges. Exact specifications, measurement temperatures and test methods are defined by the documentation of the specific manufacturer.

7. STABILITY AND FORMULATION COMPATIBILITY

The material is stable in most fragrance and functional formulations when stored correctly. Prolonged exposure to heat, moisture and strongly acidic or alkaline conditions may lead to gradual hydrolysis of the ester bond.

As an ester, it may gradually hydrolyse under the influence of moisture, elevated temperature and unfavourable formulation conditions. Compatibility, stability, colour and odour profile must be confirmed in the intended finished formulation and packaging.

8. REGULATORY DATA AND STATUS

Intended use: Professional use in fragrance, cosmetic and functional fragrance formulations.

IFRA status: Apply the current IFRA requirements and restrictions for the relevant finished-product category.

Purity requirement: As with other allyl esters, the free allyl alcohol content must be below 0.1%. Compliance must be confirmed by the specification or certificate of analysis issued by the specific manufacturer.



TECHNICAL DATA SHEET

9. STORAGE AND SHELF LIFE

Store in the original, tightly closed container in a cool, dry and dark place, protected from heat, moisture, direct sunlight and contact with air. Close the container immediately after use.

Shelf life: 24 months when stored under the recommended conditions.

10. SAFETY INFORMATION

Allyl Hexanoate is a concentrated perfumery raw material intended for professional use. It is not used on its own as a finished fragrance product and must not be applied undiluted directly to the skin.

When handling the material:

- avoid contact with skin and eyes;
- avoid ingestion and inhalation of concentrated vapours;
- wear protective gloves and eye protection;
- work in a well-ventilated area;
- keep out of reach of children.

The concentrated material may be acutely toxic if swallowed, in contact with skin or if inhaled, and may also present a hazard to the aquatic environment. The exact CLP classification and corresponding hazard statements must be taken from the current safety data sheet (SDS) for the specific product.

Gradual hydrolysis during improper storage may increase the free allyl alcohol content. Correct storage and quality control are therefore particularly important.

11. DISCLAIMER

The information in this technical data sheet relates to the described raw material and is based on the supplied and standard reference technical data. Approximate physicochemical values and indicative use levels do not replace the specification, certificate of analysis, IFRA documentation or safety data sheet issued by the specific manufacturer.

The user is responsible for verifying the identity, purity, suitability, stability, safety and regulatory compliance of the material in the intended formulation, application and target market. This document does not constitute regulatory approval or a guarantee of the properties of the finished product.